TIPS & TRICKS FOR GETTING MOST VALUE OUT OF NUMERICAL DATA

Based on a manuscript draft written with Sabrina Rüschenbaum

Lars Ole Schwen

CdE Biomodels Retreat 2017, Caldes d'Estrac/Barcelona, 2017-09-13

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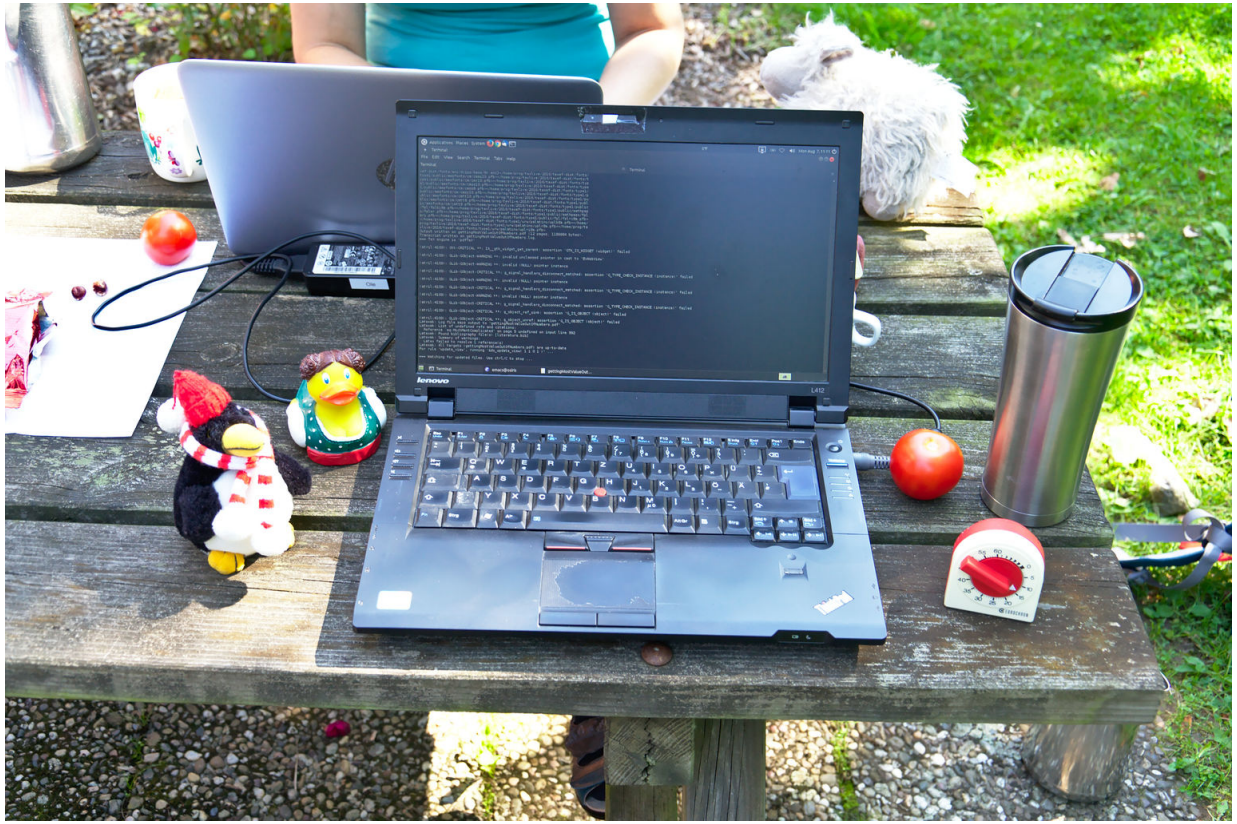
1. Introduction

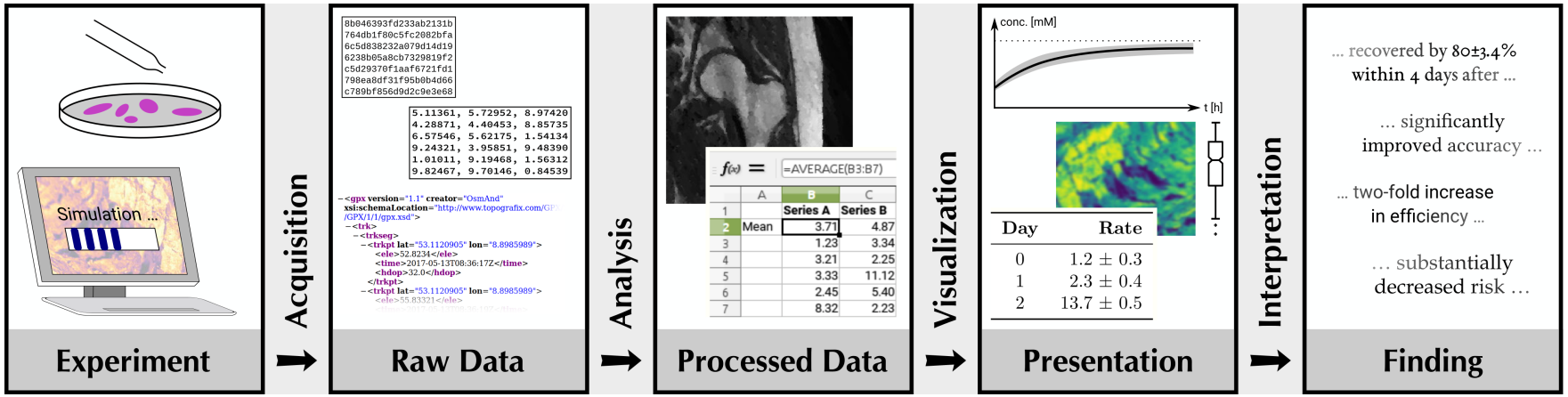
Getting Things Finished Workshop @ CdE SommerAkademie 2017



- mostly written this summer

1. Introduction

Typical Scientific Workflow



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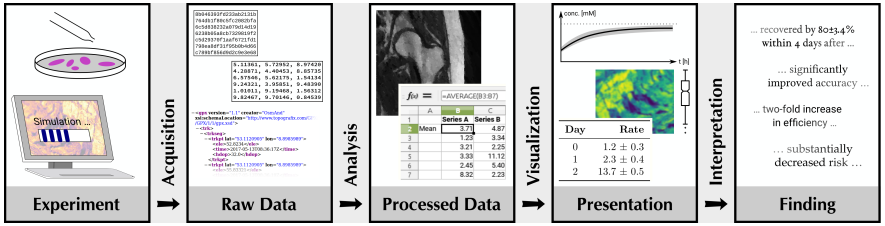
- numerical data frequently basis for findings
- acquisition, processing, and presentation need to be correct and reproducible
- mistakes are annoying, but hard to avoid
- try to make life easy for yourself and others

2. Keep Data Correct

Contents



2. Keep Data Correct

Tip 1: Plausibility-Check Your Data

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Watch out for surprising patterns

- two out of every seven values zero
- count of colony-forming units 15, 46, 28, 46, 52, and 46
- time points $t_1 = 16\,421.392\,\mathrm{s}$ and $t_2 = 20\,021.392\,\mathrm{s}$

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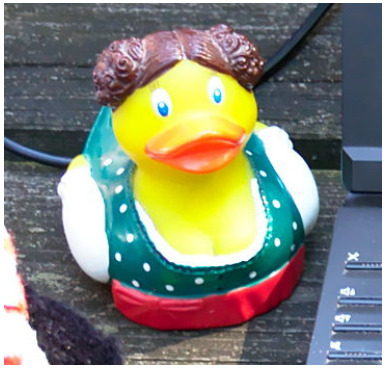
  (or explain it to your rubber duck)



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Practice guesstimation

- simplified assumptions and estimates
- back-of-the-envelope calculations
- examples below …
- Further reading: https://what-if.xkcd.com

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- budget problem or negligible?

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- observed growth of new-born Humboldt penguins for one year.

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Other example:

- Flight from Toronto to Sydney in 2.5 hours

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Pitfalls

- Undocumented way how or in which context a number was measured
- Will you find “the snail paper by Smith” in two weeks?
- Will you find $v_{\text{mean}} = 1.27$ millimeters per second if it was originally written as $V_{\text{average}} = 3$ inches per minute?

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- version-control evaluation (and manuscripts)

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- Non-finite values (NaN)

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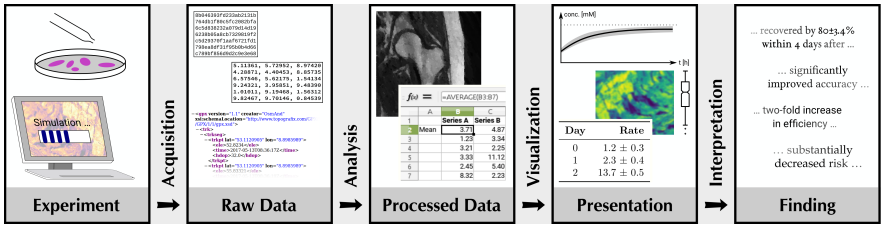

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  - summer day at 30°C in Paris
  - expect snow at 30°F in Seattle
  - superconductor experiment at 30 K

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- What is “temperature in the 30s”?
  - summer day at 30°C in Paris
  - expect snow at 30°F in Seattle
  - superconductor experiment at 30 K
- “A [mathematical] model without units is not a model.” (Matthias König)

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Tip 4: Treat Units With Respect

Use SI (Base) Units in computations

- Mistakes of factor 1000 easy to spot, 60 or 2.54 more difficult

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Caldes d’Estrac, train station

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  - 8 liters per 100 kilometers (or fuel efficiency of 29.4 miles per gallon) better

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Units in Formulas

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- integration corresponds to multiplication by unit

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Interpreting Formulas via Units

- influence of CYP enzymes on the metabolism of theobromine via Michaelis–Menten equation

$$\frac{\mathrm{d}c(t)}{\mathrm{d}t} = \dot{c}(t) = -\frac{V_{\mathrm{max}} \cdot c(t)}{K_m + c(t)} \tag{1}$$

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- factor c (concentration) in numerator implies that V_{max} has units of concentration per time, i.e., a rate of concentration change.

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Separate Unit Conversion and Formula Logic, or else …

$$\dot{c}(t) = -\frac{\frac{1\,\mathrm{min}\cdot 1\,\mathrm{mol}\cdot \tilde{V}_{\mathrm{max}}}{60\,\mathrm{s}\cdot 180.164\,\mathrm{g}} \cdot c(t)}{\frac{1\,\mathrm{min}\cdot 1\,\mathrm{mol}\cdot \tilde{K}_m}{60\,\mathrm{s}\cdot 180.164\,\mathrm{g}} + c(t)} \tag{2}$$

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- $x \to 0$
- differences $\to 0$
- denominators $\to 0$
- What is the monotonicity in these cases?

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Check Individual Constants and Variables

Recall Michaelis–Menten example:

$$\dot{c}(t) = -\frac{V_{\text{max}} \cdot c(t)}{K_m + c(t)} \tag{3}$$

V_{max} and K_m are positive constants.

- $c > 0$: negative (i.e., decrease)

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- K_m more difficult to interpret: $K_m = c$ implies half maximal rate

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Scaling

Suppose you are planning drug-drug interaction test where each drug purchase requires a lot of bureaucracy.
Effort

- *n* times purchase bureaucracy (*n* number of drugs)

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- $n(n-1)/2 = (n^2 - n)/2$ pairs of drugs (experimental effort)
- eventually, n^2 effort will dominate

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Respect Monotonicity

Suppose you quantify soil contamination based on presence of metallophytes.

✘ soil quality index (high presence $\not\Rightarrow$ high quality)

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Suppose you quantify soil contamination based on presence of metallophytes.

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✔ soil pollution index (high presence $\Rightarrow$ high pollution)

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Tip 6: Know Thy Statistical Methods

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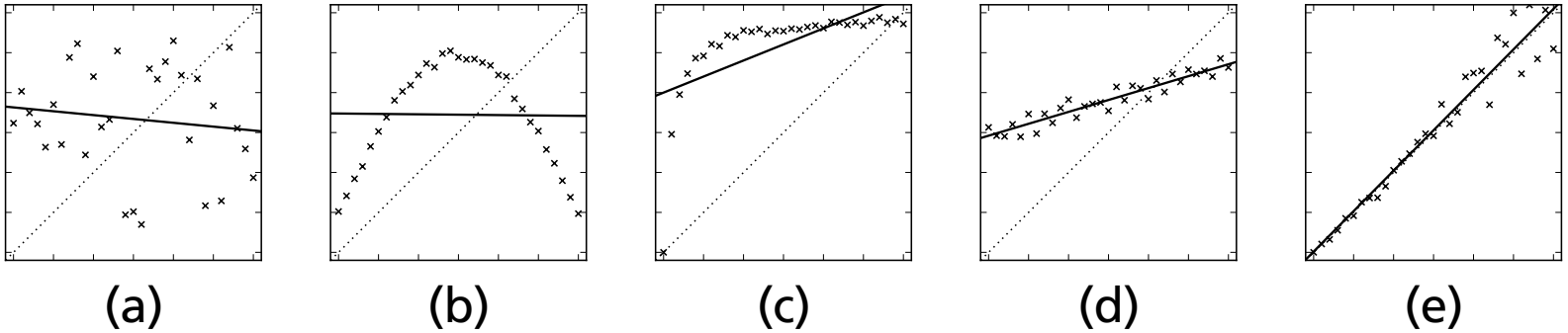
Correlation Coefficients



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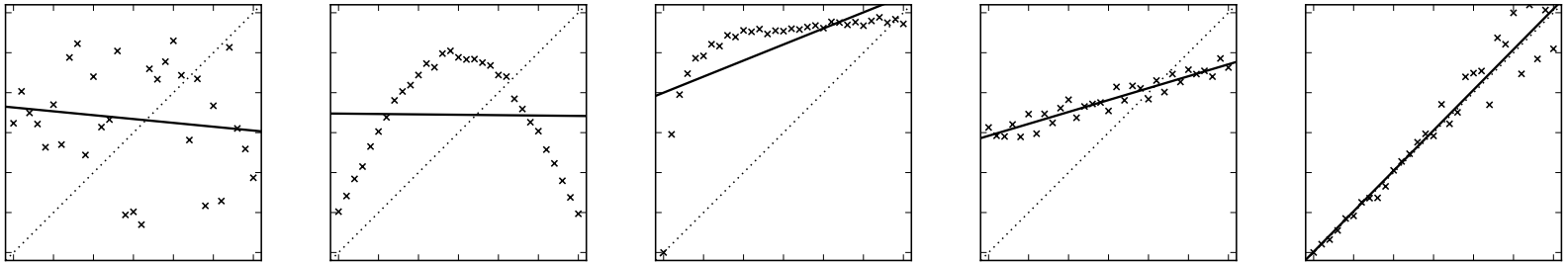

(a) (b) (c) (d) (e)

Data Series	Pearson CC
(a) noise	–0.128
(b) non-monotonic	–0.013
(c) monotonic, non-linear	0.639
(d) linear	0.948
(e) identical	0.972

- correlation is not causation, e.g., decreasing number of pirates and global warming [B. Henderson, The Gosple of the Flying Spaghetti Monster])

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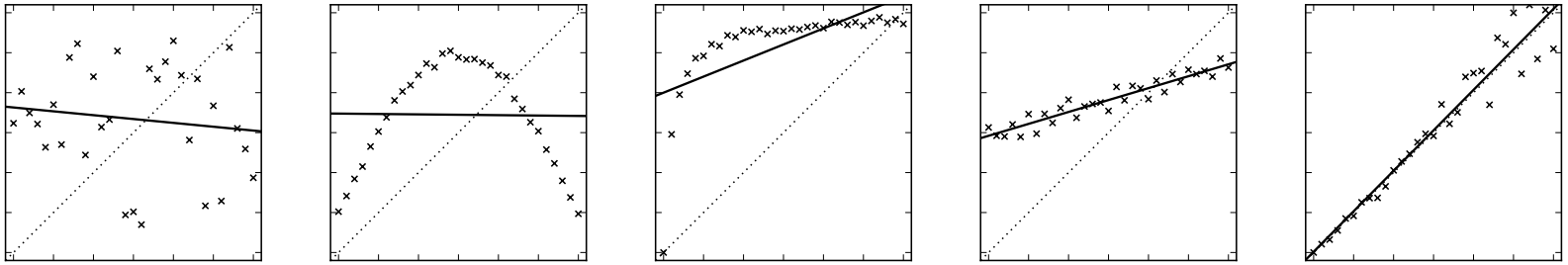

(a) (b) (c) (d) (e)

Data Series	Spearman CC	Pearson CC	Concordance CC
(a) noise	–0.108	–0.128	–0.120
(b) non-monotonic	–0.019	–0.013	–0.012
(c) monotonic, non-linear	0.955	0.639	0.280
(d) linear	0.951	0.948	0.459
(e) identical	0.971	0.972	0.971

- correlation is not causation, e.g., decreasing number of pirates and global warming [B. Henderson, The Gosple of the Flying Spaghetti Monster])

3. Correctly Interpret Your Data

Tip 6: Know Thy Statistical Methods

Statistical Significance is

✔ a high probability that an effect (e.g., difference) is not just due to randomness

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Statistical Significance is

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Statistical Significance is

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- ✘ not proof of the above
- ✘ not a measure how big the effect is
- ✘ not a measure of importance/meaning/relevance
- ✘ not a check whether the test is applicable in the first place
- ✘ lack of significance $\not\Rightarrow$ no meaningful difference

3. Correctly Interpret Your Data

Tip 6: Know Thy Statistical Methods

Analysis of the Lahman Baseball Database (Mann–Whitney *u* tests)

3. Correctly Interpret Your Data

Tip 6: Know Thy Statistical Methods

Analysis of the Lahman Baseball Database (Mann–Whitney *u* tests)

Description	Group A			Group B			approx. *p*-value
	group	*n*	Med	group	*n*	Med	
Birth Month							
b-CS	June			Sep.			1.32×10^{-4}

Med: Median, b-CS: batting/caught stealing, f-GS: fielding/games started, b-SH: batting/sacrifice hits, b-H: batting/hits, b-G: batting/games, CA: California, PA: Pennsylvania, MA: Massachusetts

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Description	Group A			Group B			approx. *p*-value
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b-CS	June	277	9.0	Sep.	348	5.0	1.32×10^{-4}

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b-CS	June	277	9.0	Sep.	348	5.0	1.32×10^{-4}
f-GS	June	471	76.0	Sep.	638	43.5	1.95×10^{-3}

Med: Median, b-CS: batting/caught stealing, f-GS: fielding/games started, b-SH: batting/sacrifice hits, b-H: batting/hits, b-G: batting/games, CA: California, PA: Pennsylvania, MA: Massachusetts

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Death Day							
b-SH	day 9	168	19.5	day 27	168	6.0	3.02×10^{-5}
b-H	day 9	248	56.5	day 27	250	23.0	3.95×10^{-5}

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Birth State							
b-G	CA	2182	121.5	PA	660	33.0	6.74×10^{-27}
b-G	CA	2182	121.5	MA	1410	52.0	1.54×10^{-25}

Med: Median, b-CS: batting/caught stealing, f-GS: fielding/games started, b-SH: batting/sacrifice hits, b-H: batting/hits, b-G: batting/games, CA: California, PA: Pennsylvania, MA: Massachusetts

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Analysis of the Lahman Baseball Database: Lessons learned

- I do not know what these baseball terms mean.

⇒ Also domain non-experts can find seemingly “highly significant” results

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- This is misuse of reasonable statistical methods for "data dredging" or "*p*-value hacking"

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Analysis of the Lahman Baseball Database: Lessons learned

- I do not know what these baseball terms mean.

⇒ Also domain non-experts can find seemingly "highly significant" results

- This is misuse of reasonable statistical methods for "data dredging" or "*p*-value hacking"
- At least, Bonferroni correction should be applied (rendering most results above non-significant)

3. Correctly Interpret Your Data

Tip 7: Keep Numbers Behind Error Bars

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- 68.432 853 percent of all statistics pretend to be more accurate than they actually are

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Error Sources and Propagation

- systematic errors, limited resolution, small samples,
- random errors (focus here)

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Error Sources and Propagation

- systematic errors, limited resolution, small samples,
- random errors (focus here)
- errors propagate through calculations
- results should not be based on noise

3. Correctly Interpret Your Data

Tip 7: Keep Numbers Behind Error Bars

Example of Uncertainty Quantification: (low-tech) measurements of ground speed of white storks

- distance 1 km ± 10 %
- time 100 s ± 1 %

3. Correctly Interpret Your Data

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Example of Uncertainty Quantification: (low-tech) measurements of ground speed of white storks

- distance 1 km ± 10 %
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- velocity uncertainty $\sqrt{10^2 + 1^2} = 10.05$ %, assuming no correlation and normal distribution
- distance error dominates

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Monte-Carlo Simulations

- repeat data evaluation many times with input data sampled from distribution estimating uncertainty

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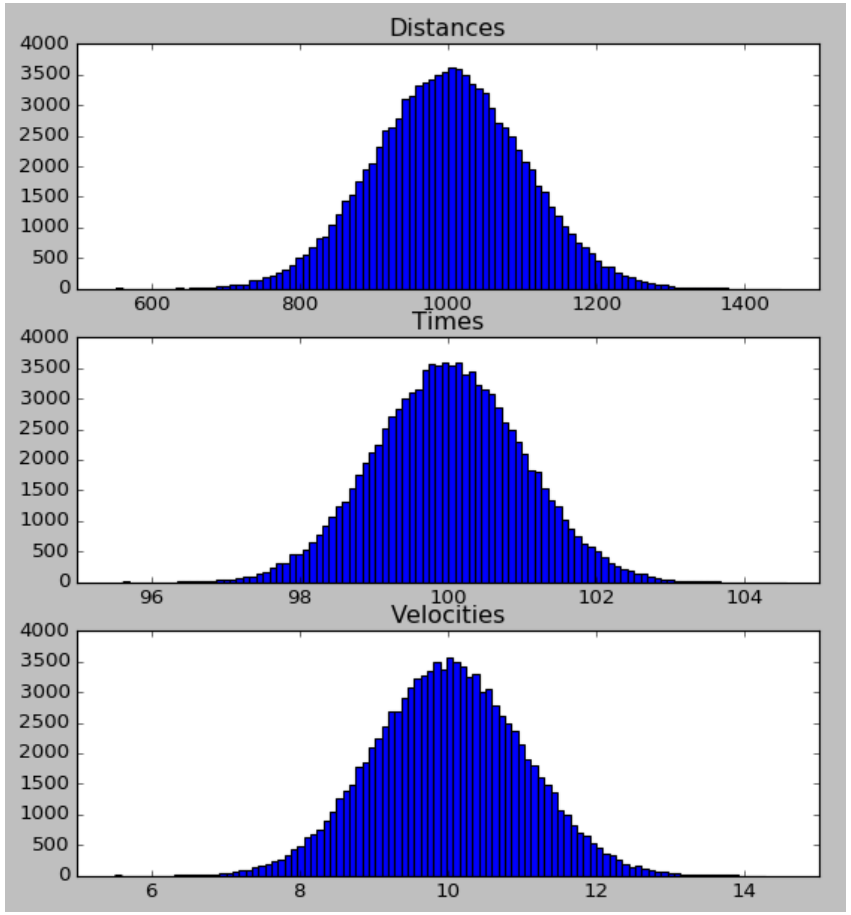

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Example of Uncertainty Quantification: (low-tech) measurements of ground speed of white storks

- distance 1 km ± 10 %
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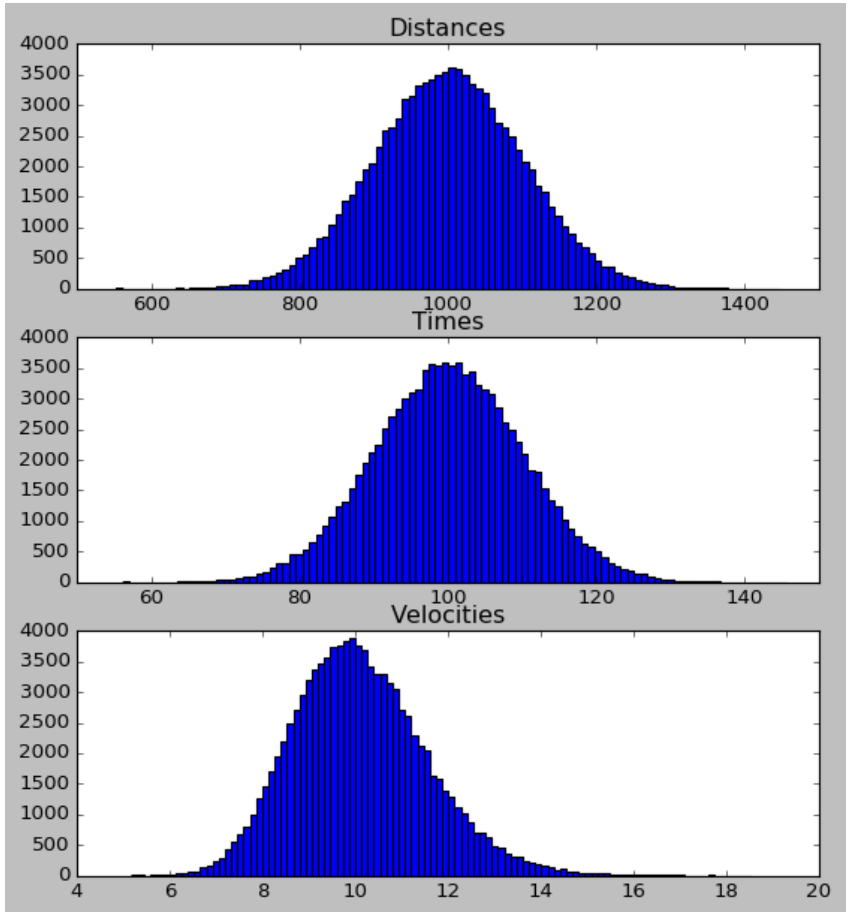
- velocity uncertainty $\sqrt{10^2 + 10^2} = 14.36\,\%$, assuming no correlation and normal distribution
- distance error dominates



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3. Correctly Interpret Your Data

Tip 8: Don’t Rely on Numbers Alone

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Tip 8: Don't Rely on Numbers Alone

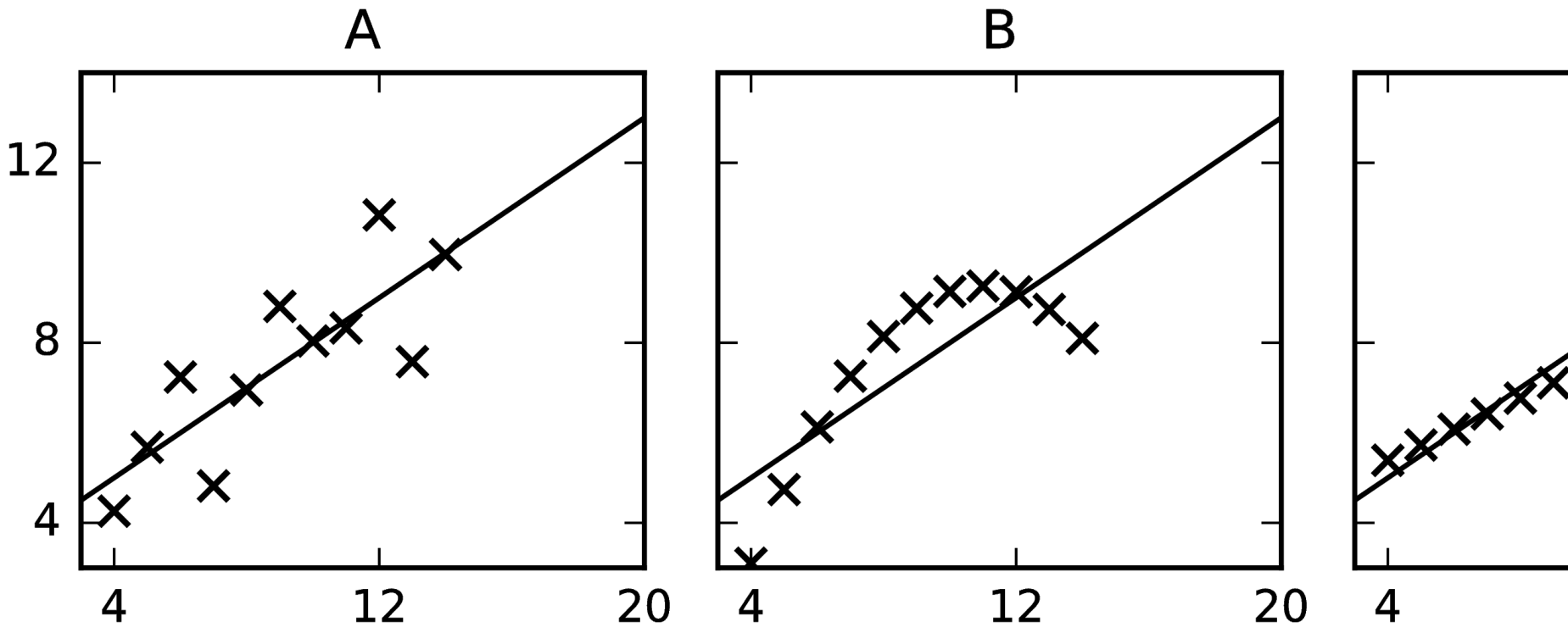
(x, y) data series A to D:

	Series A	Series B	Series C	Series D
$\bar{x}$	9.0	9.0	9.0	9.0
s_x^2	11.0	11.0	11.0	11.0
$\bar{y}$	7.5	7.5	7.5	7.5
s_y^2	4.127	4.128	4.122	4.123
$\rho_{x,y}$	0.816	0.816	0.816	0.817

- These (x, y) data series are pretty much the same. Or are they?

3. Correctly Interpret Your Data

Tip 8: Don’t Rely on Numbers Alone



- Anscombe’s quartet [Anscombe, 1973]

3. Correctly Interpret Your Data

Tip 8: Don’t Rely on Numbers Alone

Let’s count dandelions. Automatically, of course.

3. Correctly Interpret Your Data

Tip 8: Don’t Rely on Numbers Alone

Let’s count dandelions. Automatically, of course.

- Training/Calibration: This is one flower.
  Black rod (flashlight) is a length reference

3. Correctly Interpret Your Data

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Let’s count dandelions. Automatically, of course.

- Training/Calibration: This also is one flower.

3. Correctly Interpret Your Data

Tip 8: Don’t Rely on Numbers Alone

Let’s count dandelions. Automatically, of course.

Continue training and validation, maybe cross-validation …

3. Correctly Interpret Your Data

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Let’s count dandelions. Automatically, of course.

- Analysis result: 4 dandelion flowers. ??

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Tip 8: Don’t Rely on Numbers Alone

Let’s count dandelions. Automatically, of course.

- Analysis result: 5 dandelion flowers. ???

3. Correctly Interpret Your Data

Tip 8: Don’t Rely on Numbers Alone

Lessons Learned so far

- don’t blindly trust in numbers
- assess the actual data
- summarizing data is simplification and loses information

3. Correctly Interpret Your Data

Tip 8: Don’t Rely on Numbers Alone

Lessons Learned so far

- don’t blindly trust in numbers
- assess the actual data
- summarizing data is simplification and loses information

Tips:

- quick & dirty plots OK for data assessment
- choose the right way to look at it (scatter plots, time series, spatial data)

3. Correctly Interpret Your Data

Tip 8: Don’t Rely on Numbers Alone

Don’t Over-Interpret Numbers

- One number means one thing, don’t put too much meaning into it.

3. Correctly Interpret Your Data

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Don’t Over-Interpret Numbers

- One number means one thing, don’t put too much meaning into it.
  - body-mass index is not generic health measure
  - impact factor is not quality measure

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- Don’t calculate just because something is a number

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  - temperature –20°C is not “twice as cold as” –10°C

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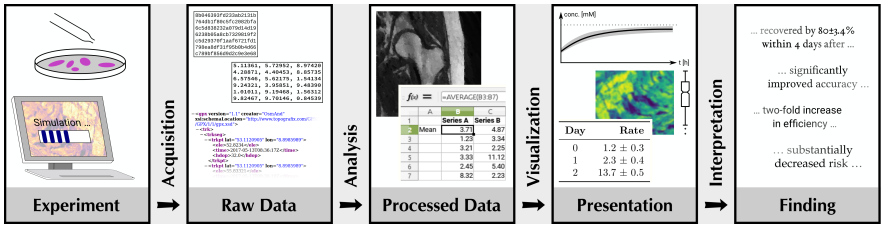
- Distinguish extensive and intensive quantities
  - 0.5 l water at 30°C and 0.5 l at 50°C is 1 l at 40°C

4. Present Your Data in a Useful Way

Contents



4. Present Your Data in a Useful Way

Tip 9: Properly Present Data

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Absolute/Relative Values/Differences

- body temperature 37.6°C (absolute)

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- body temperature 37.6°C (absolute)
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Tip 9: Properly Present Data

Absolute/Relative Values/Differences

- body temperature 37.6°C (absolute)
- overweight person (125 kg) has lost 10 kg (absolute difference)
- wheat cultivation with 20 % higher yields (relative difference)

Q: What is the baseline?

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Tip 9: Properly Present Data

How to Present Data?

- plot
  - linear vs. logarithmic
  - absolute vs. relative differences
  - interpretation of parallel lines

4. Present Your Data in a Useful Way

Tip 9: Properly Present Data

How to Present Data?

- plot—but that is not the only way
  - linear vs. logarithmic
  - absolute vs. relative differences
  - interpretation of parallel lines

4. Present Your Data in a Useful Way

Tip 9: Properly Present Data

How to Present Data?

- plot
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4. Present Your Data in a Useful Way

Tip 9: Properly Present Data

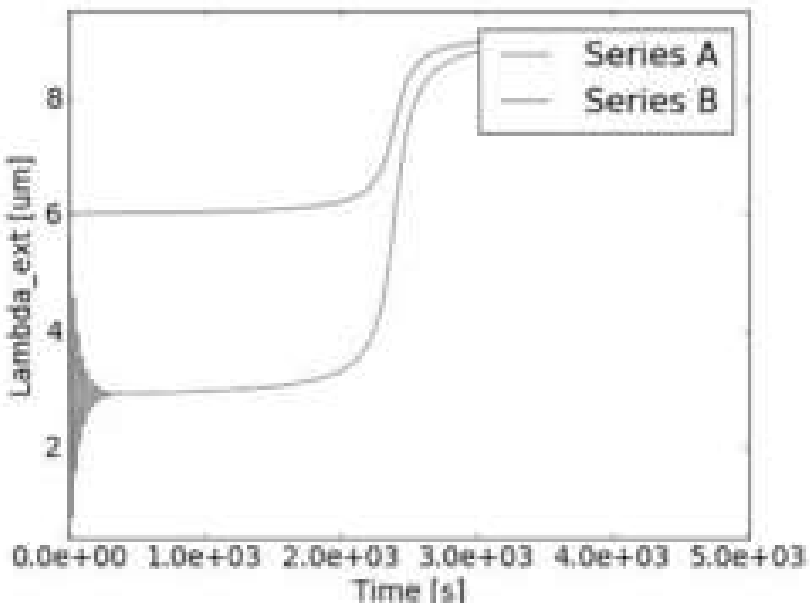
How to Present Data?

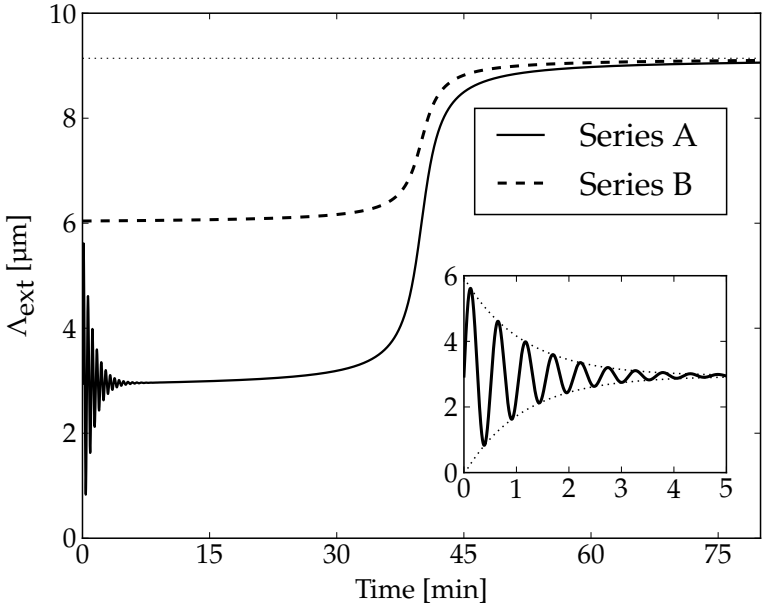
- plot
  - linear vs. logarithmic
  - absolute vs. relative differences
  - interpretation of parallel lines
- tables
- number in text
- spatial or other visualization

4. Present Your Data in a Useful Way

Tip 9: Properly Present Data

Ugly vs. Nice Plot: What is wrong on the left?





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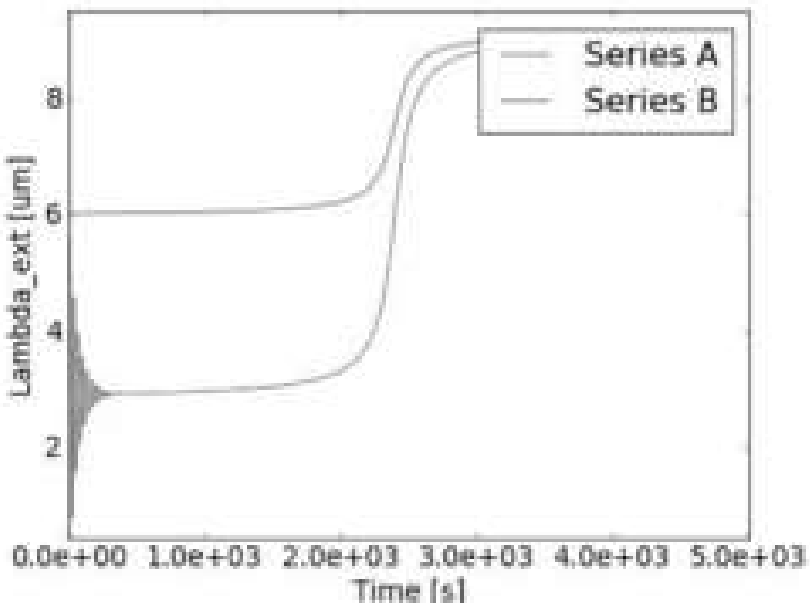
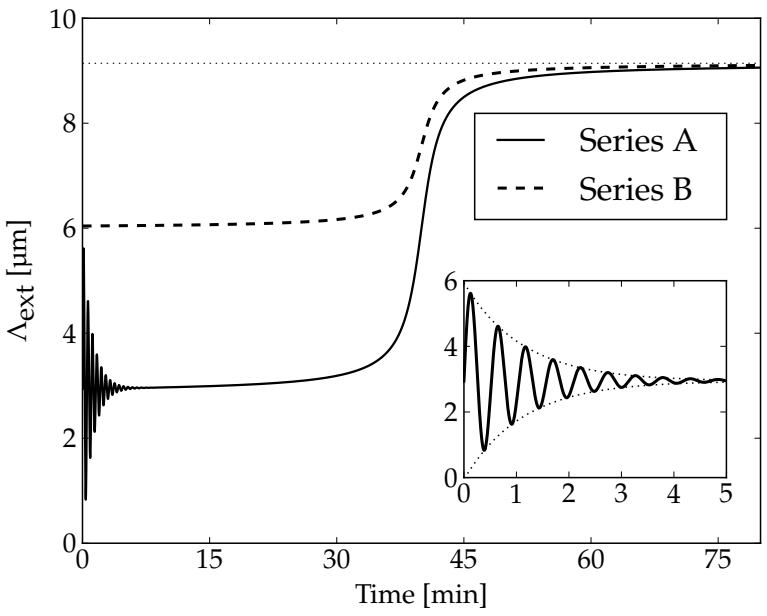


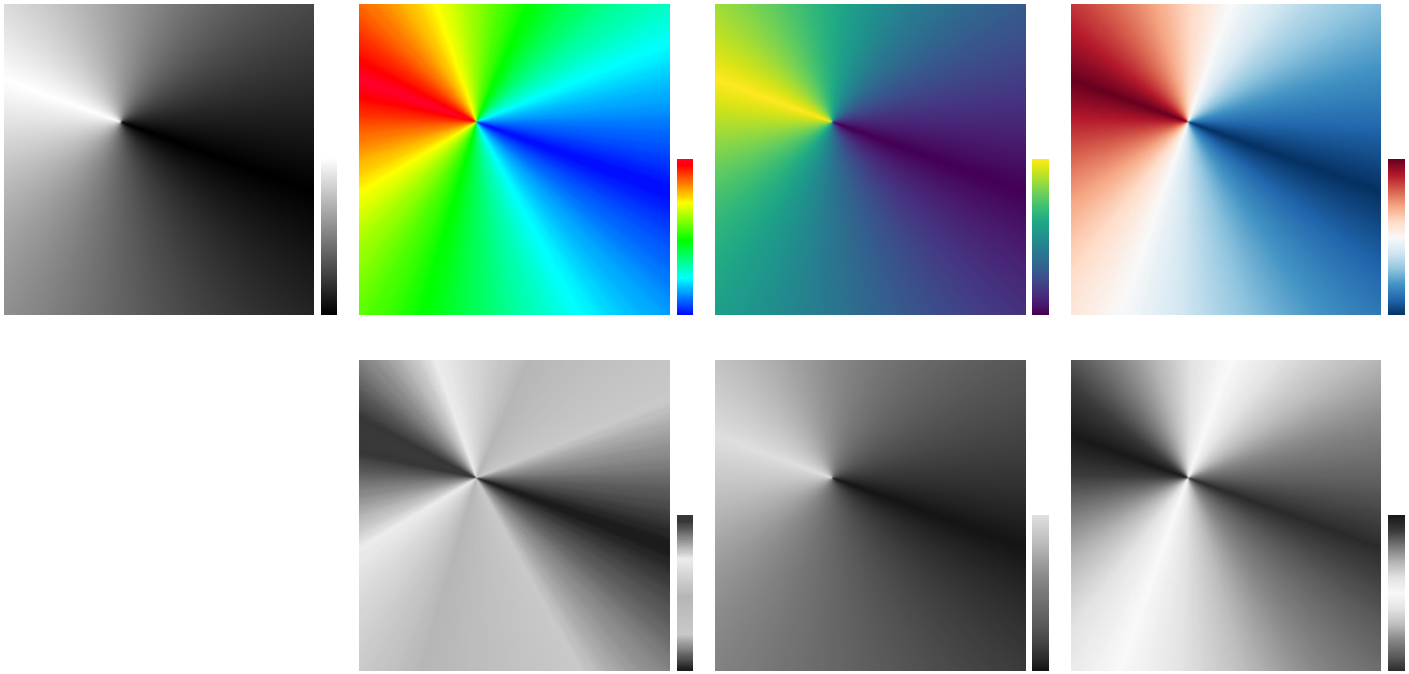


text ugly, numbers hard to read and not intuitive, curves not distinguishable, legend occludes data, oscillation not visible, value range tries but fails to start at zero, image is blurred and low-quality jpeg, relevant information missing

4. Present Your Data in a Useful Way

Tip 9: Properly Present Data

Color Scales



- distinguish sequential and divergent (and categorical) color scales
- consider color-blind people and crappy b/w printers
- avoid rainbow colormap

4. Present Your Data in a Useful Way

Tip 10: Share Your Data

4. Present Your Data in a Useful Way

Tip 10: Share Your Data

Why?

- increase credibility
- funding agencies like “open data”
- ensures long-term availability (good scientific practice)
- some journals require sharing data

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- preparing (cleaning up, standardizing, …) and documenting data may reveal mistakes

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- some journals require sharing data
- preparing (cleaning up, standardizing, …) and documenting data may reveal mistakes
- people might use the data
  - yourself at different lab
  - collaborations with others might evolve
  - others might find gems you will never go looking for

4. Present Your Data in a Useful Way

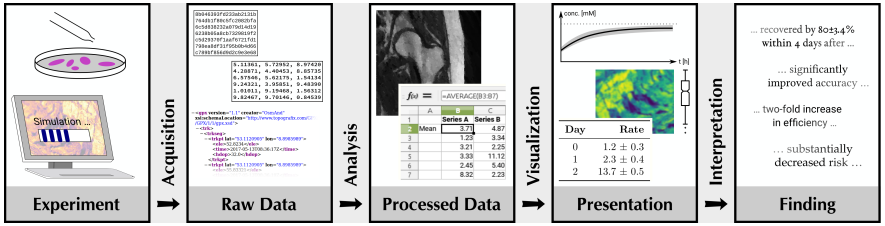
Tip 10: Share Your Data

How?

- own, institutional, project website (not optimal)
- domain-specialized or general purpose data repositories
- supporting information

5. Summary

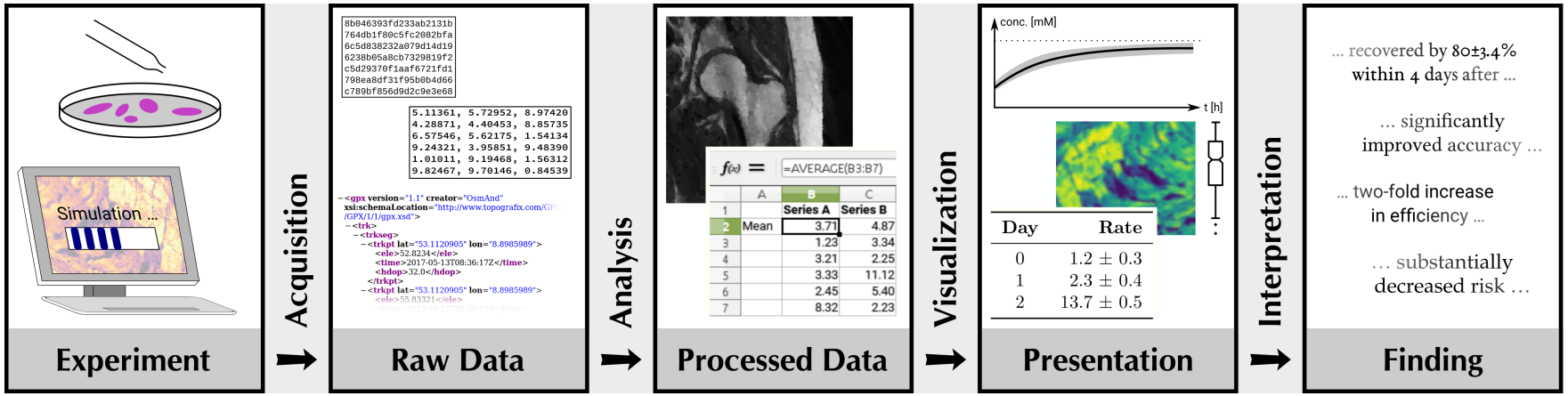
Contents



5. Summary

Tips & Tricks for Getting Most Value out of Numerical Data

1. Plausibility-Check Your Data
2. Track Your Sources
3. Beware of Computational Pitfalls
4. Treat Units With Respect
5. Verify Your Formulas
6. Know Thy Statistical Methods
7. Keep Numbers Behind Error Bars
8. Don’t Rely on Numbers Alone
9. Properly Present Data
10. Share Your Data



Contact: Ole Schwen ‹ole.schwen@mevis.fraunhofer.de›